

FAST AND SIMPLEX: 2-SIMPLICIAL ATTENTION IN TRITON

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ABSTRACT

Recent work has shown that training loss scales as a power law with both model size and the number of tokens, and that achieving compute-optimal models requires scaling model size and token count together. However, these scaling laws assume an infinite supply of data and apply primarily in compute-bound settings. As modern large language models increasingly rely on massive internet-scale datasets, the assumption that they are compute-bound is becoming less valid. This shift highlights the need for architectures that prioritize token efficiency.

In this work, we investigate the use of the 2-simplicial Transformer, an architecture that generalizes standard dot-product attention to trilinear functions through an efficient Triton kernel implementation. We demonstrate that the 2-simplicial Transformer achieves better token efficiency than standard Transformers: for a fixed token budget, similarly sized models outperform their dot-product counterparts on tasks involving mathematics, coding, reasoning, and logic. We quantify these gains by demonstrating that 2-simplicial attention changes the exponent in the scaling laws for knowledge and reasoning tasks compared to dot product attention.

1 INTRODUCTION

Large language models (LLMs) based on the Transformer architecture (Vaswani et al., 2017) have become foundational to many state-of-the-art artificial intelligence systems, including GPT-3 (Brown et al., 2020), GPT-4 (Achiam et al., 2023), Gemini (Team et al., 2023), and Llama (Touvron et al., 2023). The remarkable progress in scaling these models has been guided by neural scaling laws (Hestness et al., 2017; Kaplan et al., 2020; Hoffmann et al., 2022), which empirically establish a power-law relationship between training loss, the number of model parameters, and the volume of training data.

A key insight from this body of work is that optimal model performance is achieved not simply by increasing model size, but by scaling both the number of parameters and the amount of training data in tandem. Notably, Hoffmann et al. (2022) demonstrate that compute-optimal models require a balanced scaling approach. Their findings show that the Chinchilla model, with 70 billion parameters, outperforms the much larger Gopher model (280 billion parameters) by being trained on four times

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as much data. This result underscores the importance of data scaling alongside model scaling for achieving superior performance in large language models.

As artificial intelligence (AI) continues to advance, a significant emerging challenge is the availability of sufficiently high-quality tokens. As we approach this critical juncture, it becomes imperative to explore novel methods and architectures that can scale more efficiently than traditional Transformers under a limited token budget. However, most architectural and optimizer improvements merely shift the error but do not meaningfully change the exponent of the power law (Everett, 2025). The work of Kaplan et al. (2020); Shen et al. (2024) showed that most architectural modifications do not change the exponent, while Hestness et al. (2017) show a similar result for optimizers. The only positive result has been on data due to the works of Sorscher et al. (2022); Bahri et al. (2024); Brandfonbrener et al. (2024) who show that changing the data distribution can affect the exponent in the scaling laws.

In this context we revisit an old work Clift et al. (2019) which generalizes the dot product attention of Transformers to trilinear forms as the 2-simplicial Transformer. We explore generalizations of RoPE (Su et al., 2024) to trilinear functions and present a rotation invariant trilinear form that we prove is as expressive as 2-simplicial attention. We further show that the 2-simplicial Transformer scales better than the Transformer under a limited token budget: for a fixed number of tokens, a similar sized 2-simplicial Transformer out-performs the Transformer on math, coding and reasoning tasks. Furthermore, our experiments also reveal that the 2-simplicial Transformer has a more favorable scaling exponent corresponding to the number of parameters than the Transformer (Vaswani et al., 2017). This suggests that, unlike Chinchilla scaling (Hoffmann et al., 2022), it is possible to increase tokens at a slower rate than the parameters for the 2-simplicial Transformer. Our findings imply that, when operating under token constraints, the 2-simplicial Transformer can more effectively approach the irreducible entropy of natural language compared to dot product attention Transformers.

2 RELATED WORK

Several generalizations of attention have been proposed since the seminal work of Vaswani et al. (2017). A line of work that started immediately after was to reduce the quadratic complexity of attention with sequence length. In particular, the work of Parmar et al. (2018) proposed local attention in the context of image generation and several other works subsequently used it in conjunction with other methods for language modeling (Zaheer et al., 2020; Roy et al., 2021). Other work has proposed doing away with softmax attention altogether - e.g., Katharopoulos et al. (2020) show that replacing the softmax with an exponential without normalization leads to linear time Transformers using the associativity of matrix multiplication. Other linear time attention work are state space models such as Mamba (Gu & Dao, 2023); however these linear time attention methods have received less widespread adoption due to their worse quality compared to Transformers in practice. According to Allen (2025), the key factor contributing to Mamba’s success in practical applications is the utilization of the conv1d operator; see also So et al. (2021) and Roy et al. (2022) for similar proposals to the Transformer architecture.

The other end of the spectrum is going from quadratic to higher order attention. The first work in this direction to the best of our knowledge was 2-simplicial attention proposed by Clift et al. (2019) which showed that it is a good proxy for logical problems in the context of deep reinforcement learning. A similar generalization of Transformers was proposed in Bergen et al. (2021) which proposed the *Edge Transformer* where the authors proposed *triangular attention*. The AlphaFold (Jumper et al., 2021) paper also used an attention mechanism similar to the *Edge Transformer* which the authors called *triangle self-attention* induced by the 2D geometry of proteins. Higher order interactions were also explored in Wang et al. (2021) in the context of recommender systems. Recent work by Sanford et al. (2023) shows that the class of problems solved by an n -layer 2-simplicial Transformer is strictly larger than the class of problems solved by dot product attention Transformers. In particular, the authors define a class of problems referred to as *Match3* and show that dot product attention requires exponentially many layers in the sequence length to solve this task. Follow up work by Kozachinskiy et al. (2025) propose a scalable approximation to 2-simplicial attention and prove lowerbounds between Strassen attention and dot product attention on tasks that require more complex reasoning using VC dimension (Vapnik, 1968) arguments.

Also related is work on looping Transformer layers (Dehghani et al., 2018) as in Universal Transformers; see also Yang et al. (2023); Saunshi et al. (2025) for a more recent treatment of the same idea.

Both higher order attention and looping serve a similar purpose: compute a more expressive function per parameter. It has been established in these works that looped Transformers are better at logical reasoning tasks. A key challenge in scaling looped Transformers to larger models is their trainability. Specifically, looping k times increases the model depth by a factor of k , which can significantly exacerbate the difficulties associated with training deeper models. As a result, it remains unclear how well large looped Transformers can be trained, and further research is needed to address this concern.

Notation. We use small and bold letters to denote vectors, capital letters to denote matrices and tensors and small letters to denote scalars. We denote $\langle \mathbf{a}, \mathbf{b} \rangle$ to denote dot product between two vectors \mathbf{a} and \mathbf{b} . Similarly, the trilinear dot product is denoted as follows: $\langle \mathbf{a}, \mathbf{b}, \mathbf{c} \rangle = \sum_{i=1}^d \langle \mathbf{a}_i, \mathbf{b}_i, \mathbf{c}_i \rangle$. We use $\textcircled{\cdot}$ to highlight a matrix multiplication, for e.g., $(AB)\textcircled{C}$, for matrices A, B, C . To denote array slicing, we use $\mathbf{a}[l : l + m] = (a_l, \dots, a_{l+m-1})$ with zero-based indexing. Some tensor operations are described using Einstein summation notation as used in the Numpy library (Harris et al., 2020). We use *FLOPs* to denote floating point operations. Column stacking of arrays are denoted by $[\mathbf{a}, \mathbf{b}, \mathbf{c}]$. We use \det to denote determinant of a square matrix.

3 OVERVIEW OF NEURAL SCALING LAWS

In this section we provide a brief overview of neural scaling laws as introduced in Kaplan et al. (2020). We will adopt the approach outlined by Hoffmann et al. (2022), which proposes that the loss $L(N, D)$ decays as a power law in the total number of model parameters N and the number of tokens D :

$$L(N, D) = E + \frac{A}{N^\alpha} + \frac{B}{D^\beta}. \quad (1)$$

The first term E is often described as the *irreducible loss* which corresponds to the entropy of natural text. The second term captures the fact that a model with N parameters underperforms this ideal generative process. The third term corresponds to the fact that we train on only a finite sample of the data and do not train the model to convergence. Theoretically, as $N \rightarrow \infty$ and $D \rightarrow \infty$ a large language model should approach the irreducible loss E of the underlying text distribution.

For a given compute budget C where $\text{FLOPs}(N, D) = C$, one can express the optimal number of parameters as $N_{\text{opt}} \propto C^a$ and the optimal dataset size as $D_{\text{opt}} \propto C^b$. The authors of Hoffmann et al. (2022) perform several experiments and fit parametric functions to the loss to estimate the exponents a and b : multiple different approaches confirm that roughly $a \sim 0.49$ while $b \sim 0.5$. This leads to the central thesis of Hoffmann et al. (2022): one must scale the number of tokens proportionally to the model size.

However, as discussed in Section 1, the quantity of sufficiently high-quality tokens is an emerging bottleneck in pre-training scaling, necessitating an exploration of alternative training algorithms and architectures. On the other hand recent studies have shown that most modeling and optimization techniques proposed in the literature merely shift the error (offset E) and do not fundamentally change the exponent in the power law. We refer the readers to this excellent discussion in Everett (2025).

4 THE 2-SIMPLICIAL TRANSFORMER

The 2-simplicial Transformer was introduced in Clift et al. (2019) where the authors extended the dot product attention from bilinear to trilinear forms, or equivalently from the 1-simplex to the 2-simplex. Let us recall the attention mechanism in a standard Transformer (Vaswani et al., 2017). Given a sequence $X \in \mathbb{R}^{n \times d}$ we have three projection matrices $W_Q, W_K, W_V \in \mathbb{R}^{d \times d}$ which we refer to as the query, key and value projections respectively. These projection matrices are used to infer the query $Q = XW_Q$, key $K = XW_K$ and value $V = XW_V$ respectively. This is then used to construct the *attention logits*:

$$A = QK^\top / \sqrt{d} \in \mathbb{R}^{n \times n}, \quad (2)$$

where each entry is a dot product $A_{ij} = \langle \mathbf{q}_i, \mathbf{k}_j \rangle / \sqrt{d}$ which are both entries in \mathbb{R}^d . The attention scores (logits) are then transformed into probability weights by using a row-wise softmax operation:

$$S_{ij} = \exp(A_{ij}) / \sum_{j=1}^n \exp(A_{ij}). \quad (3)$$

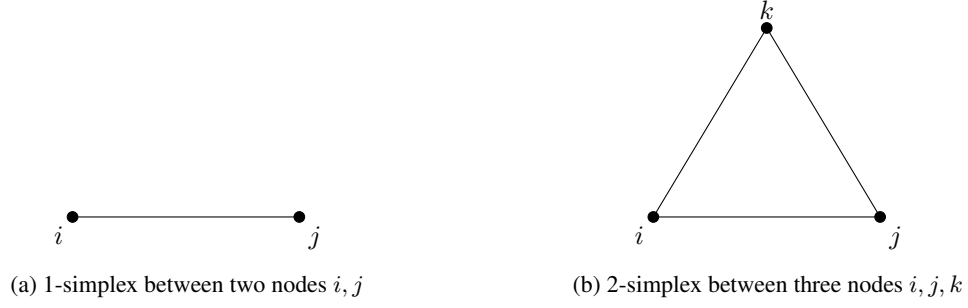


Figure 1: Geometry of dot product attention and 2-simplicial attention.

The final output of the attention layer is then a linear combination of the values according to these attention scores:

$$\tilde{v}_i = \sum_{j=1}^n A_{ij} v_j \quad (4)$$

The 2-simplicial Transformer paper [Clift et al. \(2019\)](#) generalizes this to trilinear products where we have two additional key and value projection matrices $W_{K'}$ and $W_{V'}$, which give us $K' = XW_{K'}$ and $V' = XW_{V'}$. The attention logits for 2-simplicial Transformer are then given by the trilinear product between Q , K and K' , resulting in the following third-order tensor:

$$A_{ijk}^{(2s)} = \frac{\langle \mathbf{q}_i, \mathbf{k}_j, \mathbf{k}'_k \rangle}{\sqrt{d}} = \frac{1}{\sqrt{d}} \sum_{l=1}^d Q_{il} K_{jl} K'_{kl}, \quad (5)$$

so that the attention tensor becomes:

$$S_{ijk}^{(2s)} = \exp(A_{ijk}^{(2s)}) / \sum_{j,k} \exp(A_{ijk}^{(2s)}), \quad (6)$$

with the final output of the attention operation being defined as

$$\tilde{v}^{(2s)}(i) = \sum_{j,k=1}^n S_{ijk}^{(2s)} (v_j \circ v'_k), \quad (7)$$

where $v_j \circ v'_k$ represents the element wise Hadamard product between two vectors in \mathbb{R}^d . The pseudo-code for 2-simplicial attention is depicted in Algorithm 1. Note that Equation 5 does not incorporate any position encoding such as RoPE ([Su et al., 2024](#)); we discuss this in the next section.

Algorithm 1 Pseudocode for the forward pass of 2-simplicial attention

- 1: **procedure** 2-SIMPLICIAL ATTENTION(Q, K, V, K', V')
 - 2: logits \leftarrow einsum(“b_{tnh}, b_{snh}, b_{rnh} \rightarrow b_{ntsr}”, Q, K, K')
 - 3: attention \leftarrow softmax(logits + causal-mask, axis = $[-1, -2]$)
 - 4: output \leftarrow einsum(“b_{ntsr}, b_{snh}, b_{rnh} \rightarrow b_{tnh}”, attention, V, V')
 - 5: **return** output
 - 6: **end procedure**
-

5 DETERMINANT BASED TRILINEAR FORMS

RoPE ([Su et al., 2024](#)) was proposed as a way to capture the positional information in a sequence for Transformer language models. RoPE applies a position dependent rotation to the queries \mathbf{q}_i and the key \mathbf{k}_j so that the dot product $\langle \mathbf{q}_i, \mathbf{k}_j \rangle$ is a function of the relative distance $i - j$. In particular, note that the dot product is invariant to orthogonal transformations $R \in \mathbb{R}^{d \times d}$:

$$\langle \mathbf{q}_i, \mathbf{k}_j \rangle = \langle R\mathbf{q}_i, R\mathbf{k}_j \rangle.$$

This is important for RoPE to work as for a query \mathbf{q}_i and key \mathbf{k}_i at the same position i , we expect its dot product to be unchanged by the application of position based rotations: $\langle \mathbf{q}_i, \mathbf{k}_i \rangle = \langle R\mathbf{q}_i, R\mathbf{k}_i \rangle$.

Note that the trilinear form defined in Equation 5 is not invariant to rotation and the application of the same rotation to \mathbf{q}_i , \mathbf{k}_i and \mathbf{k}'_i no longer preserves the inner product: $\langle \mathbf{q}_i, \mathbf{k}_i, \mathbf{k}'_i \rangle = \sum_{l=1}^d \mathbf{q}_{il} \mathbf{k}_{il} \mathbf{k}'_{il} \neq \langle R\mathbf{q}_i, R\mathbf{k}_i, R\mathbf{k}'_i \rangle$. Therefore, to generalize RoPE to 2-simplicial attention, it is important to explore alternative bilinear and trilinear forms that are rotation invariant.

We note that the following functions are also invariant to rotations:

$$\begin{aligned} \hat{f}_2(\mathbf{a}, \mathbf{b}) &= \det \begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} = a_1 b_2 - a_2 b_1, \\ \hat{f}_3(\mathbf{a}, \mathbf{b}, \mathbf{c}) &= \det \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}, \\ &= a_1 b_2 c_3 + a_2 b_3 c_1 + a_3 b_1 c_2 - a_1 b_3 c_2 - a_2 b_1 c_3 - a_3 b_2 c_1 \\ &= \langle (a_1, a_2, a_3), (b_2, b_3, b_1), (c_3, c_1, c_2) \rangle - \langle (a_1, a_2, a_3), (b_3, b_1, b_2), (c_2, c_3, c_1) \rangle, \quad (8) \end{aligned}$$

the rearrangement in the last equality is popularly called Sarrus rule (Strang, 2022). Here, \hat{f}_2 is a bilinear form in $\mathbf{a} = (a_1, a_2)$ and $\mathbf{b} = (b_1, b_2)$ and \hat{f}_3 is a trilinear form in $\mathbf{a} = (a_1, a_2, a_3)$, $\mathbf{b} = (b_1, b_2, b_3)$, $\mathbf{c} = (c_1, c_2, c_3)$. Geometrically, $|\hat{f}_2(\mathbf{a}, \mathbf{b})|$ measures the area of the parallelogram spanned by \mathbf{a} and \mathbf{b} , and similarly, $|\hat{f}_3(\mathbf{a}, \mathbf{b}, \mathbf{c})|$ measures the volume of the parallelotope spanned by \mathbf{a} , \mathbf{b} and \mathbf{c} . We use the signed determinant operation \hat{f}_3 to compute $A^{(\det)} \in \mathbb{R}^{n \times n \times n}$. For any vector \mathbf{q} , let $\mathbf{q}^{(l)} = \mathbf{q} = \mathbf{q}[3(l-1) : 3l]$ be its l th chunk of size 3. The logits are defined as:

$$A_{ij_1 j_2}^{(\det)} = \sum_{l=1}^p \det([\mathbf{q}_i^{(l)}, \mathbf{k}_{j_1}^{(l)}, \mathbf{k}'_{j_2}{}^{(l)}]). \quad (9)$$

Since Equation 8 has 2 dot product terms due to Sarrus rule, it would modify Algorithm 1 to use 2 einsums instead of 1 in line 2. The final attention weights S are computed by applying a softmax function on the logits above, similar to Equation 6. The output for token i is then the weighted sum of value vectors as in Equation 7.

Theorem 5.1. *For any input size n and input range $m = n^{O(1)}$, there exists a transformer architecture with a single head of attention with logits computed as in (9), with attention head dimension $d = 7$, such that for all $X \in [M]^N$, the transformer’s output for element x_i is 1 if $\exists j_1, j_2$ s.t. $x_i + x_{j_1} + x_{j_2} = 0 \pmod{M}$, and 0 otherwise.*

We provide the proof in Appendix A. Since the sum-of-determinants trilinear function of Equation 9 involves 6 terms compared to the simpler trilinear form of Equation 5, in the following sections where we compute the backwards function for 2-simplicial attention, we will use the simpler trilinear form of Equation 5 without loss of generality.

6 MODEL DESIGN

Since 2-simplicial attention scales as $\mathcal{O}(n^3)$ in the sequence length n , it is impractical to apply it over the entire sequence. Instead, we parametrize it as $\mathcal{O}(n \times w_1 \times w_2)$, where w_1 and w_2 define the dimensions of a sliding window over the sequence. Each query vector Q_i attends to a localized region of w_1 K keys and w_2 K' keys, thereby reducing the computational burden. We systematically evaluate various configurations of w_1 and w_2 to identify optimal trade-offs between computational efficiency and model performance (see Table 1).

For causal dot product attention, the complexity for a sequence of length n is given by:

$$O(A) = \frac{1}{2} \cdot 2 \cdot 2n^2 = 2n^2,$$

where n is the sequence length. This involves two matrix multiplications: one for $Q@K$, one for $P@V$, each requiring two floating-point operations per element. The causal mask allows us to skip $\frac{1}{2}$ of these computations.

In contrast, the complexity of 2-simplicial attention, parameterized by w_1 and w_2 , is expressed as:

$$O(A^{(2s)}) = 3 \cdot 2nw_1w_2 = 6nw_1w_2$$

This increase in complexity arises from the trilinear einsum operation, which necessitates an additional multiplication compared to standard dot product attention.

$w_1 \times w_2$	w_1	w_2	Latency (ms)
32k	1024	32	104.1 ms
32k	512	64	110.7 ms
16k	128	128	59.2 ms
16k	256	64	55.8 ms
16k	512	32	55.1 ms
16k	1024	16	55.1 ms
8k	256	32	28.3 ms

Table 1: Latency for different combinations of w_1, w_2

We choose a window size of (512, 32), balancing latency and quality. With this configuration, the computational complexity of 2-simplicial attention is comparable to dot product attention at 48k context length.

A naive sliding window 2-simplicial attention implementation has each Q_i vector attending to $w_1 + w_2 - 1$ different KK' vectors, as illustrated in Figure 2. Thus, tiling queries Q like in flash attention leads to poor compute throughput. Inspired by Native Sparse Attention (Yuan et al., 2025), we adopt a model architecture leveraging a high Grouped Query Attention GQA (Ainslie et al., 2023) ratio of 64. This approach enabled efficient tiling along query heads, ensuring dense computation and eliminating the need for costly element-wise masking.

7 KERNEL OPTIMIZATION

We introduce a series of kernel optimizations tailored for 2-simplicial attention, building off of Flash Attention (Dao et al., 2022) using online softmax. For the trilinear operations, we perform 2d tiling by merging one of the inputs via elementwise multiplication and executing matmul on the product as illustrated in Figure 2. This allows us to overlap both QK and VV' on CUDA Core with $(QK)@K'$ and $P@(VV')$ on Tensor Core. Implementing this in Triton, we achieve 520 TFLOPS, rivaling the fastest FAv3 Triton implementations. Further optimization could be achieved with a lower-level language like CUTLASS for finer grained tuning and optimizations. Despite this, we achieve competitive performance compared to CUTLASS FAv3 for large sequence lengths, as shown in Figure 3.

For the backwards pass, we have

$$dV_{jd} = \sum_{i,k} (A_{ijk} \cdot dO_{id} \cdot V'_{kd}) \quad (10)$$

$$dV'_{kd} = \sum_{i,j} (A_{ijk} \cdot dO_{id} \cdot V_{jd}) \quad (11)$$

$$dP_{ijk} = \sum_d (dO_{id} \cdot V_{jd} \cdot V'_{kd}) \quad (12)$$

$$dS = d\text{softmax}_{jk}(dP) \quad (13)$$

$$dK_{jd} = \sum_{i,k} (Q_{id} \cdot dS_{ijk} \cdot K'_{kd}) \quad (14)$$

$$dK'_{kd} = \sum_{i,k} (Q_{id} \cdot dS_{ijk} \cdot K_{jd}) \quad (15)$$

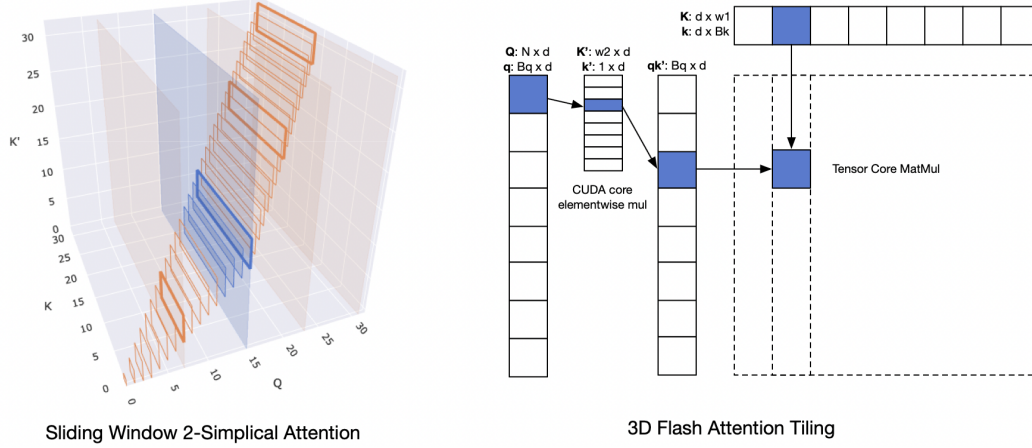


Figure 2: **Left:** Visualization of sliding window 2-simplicial attention. Each Q_i attends to a $[w1, w2]$ shaped rectangle of K, K' . **Right:** Tiling to reduce 2-simplicial einsum $QK'K'$ to elementwise mul QK' on CUDA core and tiled matmul $(QK')@K$ on tensor core.

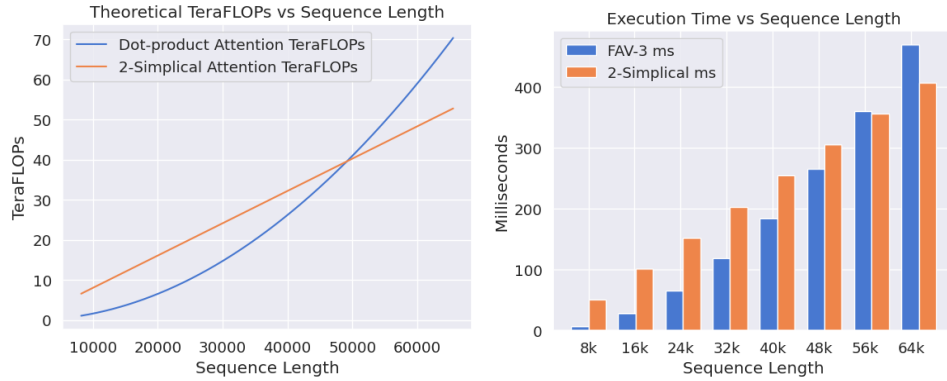


Figure 3: FLOPs and Latencies of FAV3 vs 2-simplicial attention

$$dQ_{id} = \sum_{j,k} (dS_{ijk} \cdot K_{jd} \cdot K'_{kd}) \quad (16)$$

For the backwards pass, aggregations across three different dimension orderings introduces significant overhead from atomic operations. To mitigate this, we decompose the backward pass into two distinct kernels: one for computing dK and dV , and another for dK' , dV' , and dQ . Although this approach incurs additional overhead from recomputing O and dS , we find it is better than the extra overhead from atomics needed for a single fused kernel. We note this may be a limitation of Triton’s coarser grained pipeline control making it difficult to hide the overhead from atomics.

For small w_2 , we employ a two-stage approach to compute dQ jointly with dK' , dV' without atomics as detailed in Algorithm 2. We divide Q along the sequence dimension into

$$\lceil w_2, dim \rceil$$

sized tiles. First we iterate over even tiles, storing dQ , dK , dK' , and dV , dV' . Then we iterate over odd tiles, storing dQ , and adding to dK , dK' and dV , dV' .

Algorithm 2 Backward pass for 2-simplicial attention

```

1: procedure 2-SIMPLICIAL FLASH ATTENTION BWD( $Q, K, V, K', V', w_1, w_2$ )
2:   for stage in  $[0, 1]$  do
3:     for q_start in range(stage *  $w_2$ , seq_len,  $w_2 * 2$ ) do
4:       q_end  $\leftarrow$  q_start +  $w_2$ 
5:       for kv1_start in range(q_start -  $w_1$ , q_end) do
6:         q_tile  $\leftarrow$   $Q[q\_start : q\_end]$ 
7:         ...
8:         k2_tile  $\leftarrow$   $K'[kv1\_start : q\_end]$ 
9:          $dQ \mathrel{+}= dQ(q\_tile, k2\_tile, \dots)$ 
10:         $dV' \mathrel{+}= dV'(q\_tile, k2\_tile, \dots)$ 
11:         $dK' \mathrel{+}= dK'(q\_tile, k2\_tile, \dots)$ 
12:      end for
13:      if stage == 1 then
14:         $dK' \mathrel{+}= \text{load } dK'$ 
15:         $dV' \mathrel{+}= \text{load } dV'$ 
16:      end if
17:      store  $dQ, \dots, dK'$ 
18:    end for
19:  end for
20: end procedure

```

8 EXPERIMENTS & RESULTS

We train a series of MoE models (Jordan & Jacobs, 1994; Shazeer et al., 2017) ranging from 1 billion active parameters and 57 billion total parameters to 3.5 billion active parameters and 176 billion total parameters. We use interleaved sliding-window 2-simplicial attention, where every fourth layer is a 2-simplicial attention layer. The choice of this particular ordering is to distribute the load in attention computation when using pipeline parallelism (Huang et al., 2019; Narayanan et al., 2019), since 2-simplicial attention and global attention are the most compute intensive operations in a single pipeline stage and have comparable FLOPs.

We use the AdamW optimizer (Loshchilov et al., 2017) with a peak learning rate of 4×10^{-3} and weight decay of 0.0125. We use a warmup of 4000 steps and use a cosine decay learning schedule decreasing the learning rate to $0.01 \times$ of the peak learning rate. We report the negative log-likelihood on GSM8k (Cobbe et al., 2021), MMLU (Hendrycks et al., 2020), MMLU-pro (Wang et al., 2024) and MBPP (Austin et al., 2021), since these benchmarks most strongly test math, reasoning and coding skills in pre-training.

Model	Active Params	Total Params	GSM8k	MMLU	MMLU-pro	MBPP
Transformer	1B	57B	0.3277	0.6411	0.8718	0.2690
2-simplicial	1B	57B	0.3302	0.6423	0.8718	0.2714
$\Delta(\%)$			+0.79%	+0.19%	-0.01%	+0.88%
Transformer	2B	100B	0.2987	0.5932	0.8193	0.2435
2-simplicial	2B	100B	0.2942	0.5862	0.8135	0.2411
$\Delta(\%)$			-1.51%	-1.19%	-0.71%	-1%
Transformer	3.5B	176B	0.2781	0.5543	0.7858	0.2203
2-simplicial	3.5B	176B	0.2718	0.5484	0.7689	0.2193
$\Delta(\%)$			-2.27%	-1.06%	-2.15%	-0.45%

Table 2: Negative log-likelihood of Transformer (Vaswani et al., 2017) versus 2-simplicial attention. For MMLU (Hendrycks et al., 2020) and MMLU-pro (Wang et al., 2024) we measure the negative log-likelihood of the choice together with the entire answer. For GSM8k (Cobbe et al., 2021) we use 5-shots for the results.

We see that the decrease (Δ) in negative log-likelihood scaling from a 1.0 billion (active) parameter model increases going to a 3.5 billion (active) parameter model. Furthermore, on models smaller than 2.0 billion (active) parameters, we see no gains from using 2-simplicial attention. From Table 2 we can estimate how the power law coefficients for the 2-simplicial attention differ from dot product attention. Recall from Section 3 that the loss can be expressed as:

$$L(N, D) = E + \frac{A}{N^\alpha} + \frac{B}{D^\beta}. \quad (17)$$

Since we train both the models on the same fixed number of tokens, we may ignore the third term and simply write the loss as:

$$L(N) = E' + \frac{A}{N^\alpha}, \quad (18)$$

$$\log L(N) \approx \log E'' + \log A - \alpha \log N \quad (19)$$

$$-\log L(N) = \alpha \log N + \beta, \quad (20)$$

where $\beta = -\log E'' - \log A$ and E'' is an approximation to E' since E' is small. Note that here we used $\log(a + b) = \log(1 + a/b) + \log(b)$ to separate out the two terms, with the $1 + a/b$ term hidden in E'' . Therefore we can estimate α, β for both sets of models from the losses in Table 2 where we use for N the active parameters in each model. We estimate the slope α and the intercept β for both the Transformer as well as the 2-simplicial Transformer in Table 3. We see that 2-simplicial attention has a steeper slope α , i.e. a higher exponent in its scaling law compared to dot product attention Transformer (Vaswani et al., 2017).

Model	GSM8k		MMLU		MMLU-pro		MBPP	
	α	β	α	β	α	β	α	β
Transformer	0.1420	-1.8280	0.1256	-2.1606	0.0901	-1.7289	0.1720	-2.2569
2-simplicial	0.1683	-2.3939	0.1364	-2.3960	0.1083	-2.1181	0.1837	-2.5201
$\Delta(\%)$	18.5%		8.5%		20.2%		6.8%	

Table 3: Estimates of the power law coefficients α and β for the Transformer (Vaswani et al., 2017) and 2-simplicial attention.

Model	GSM8k		MMLU		MMLU-pro		MBPP	
	R^2	residual	R^2	residual	R^2	residual	R^2	residual
Transformer	0.9998	2.8×10^{-6}	0.9995	4.7×10^{-6}	0.9972	1.5×10^{-5}	0.9962	7.5×10^{-5}
2-simplicial	0.9974	4.9×10^{-5}	0.9989	1.3×10^{-5}	0.9999	4.6×10^{-8}	0.9999	1.5×10^{-6}

Table 4: R^2 and residuals measuring goodness of fit for Table 3.

9 DISCUSSION

While 2-simplicial attention improves the exponent in the scaling laws, we should caveat that the technique maybe more useful when we are in the regime when token efficiency becomes more important. Our Triton kernel while efficient for prototyping is still far away from being used in production. More work in co-designing the implementation of 2-simplicial attention tailored to the specific hardware accelerator is needed in the future.

10 CONCLUSION

We show that a similar sized 2-simplicial attention (Clift et al., 2019) improves on dot product attention of Vaswani et al. (2017) by improving the negative log likelihood on reasoning, math and coding problems (see Table 2). We quantify this explicitly in Table 3 by demonstrating that 2-simplicial attention changes the exponent corresponding to parameters in the scaling law of Equation 18: in particular it has a higher α for reasoning and coding tasks compared to the Transformer (Vaswani et al., 2017) which leads to more favorable scaling under token constraints. Furthermore, the percentage increase in the scaling exponent α is higher for less saturated and more challenging benchmarks such as MMLU-pro and GSM8k.

We hope that scaling 2-simplicial Transformers could unlock significant improvements in downstream performance on reasoning-heavy tasks, helping to overcome the current limitations of pre-training scalability. Furthermore, we believe that developing a specialized and efficient implementation is key to fully unlocking the potential of this architecture.

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A ROTATION INVARIANT TRILINEAR FORMS

A.1 PROOF FOR THEOREM 5.1

We define the embedding functions for the Query and Key vectors such that their interaction within the Sum-of-Determinants attention mechanism computes the `Match3` function. To handle cases where no match exists, we use a 7-dimensional embedding where the 7th dimension acts as a selector for a "blank pair" option, a technique adapted from `Match2` construction in [Sanford et al. \(2023\)](#).

The construction for regular token pairs is based on the mathematical identity:

$$\cos(\theta_1 + \theta_2 + \theta_3) = \det(M_1) + \det(-M_2), \quad (21)$$

where the matrices $M_1, M_2 \in \mathbb{R}^{3 \times 3}$ are defined as:

$$M_1 = \begin{pmatrix} \cos(\theta_1) & \sin(\theta_1) & 0 \\ \sin(\theta_2) & \cos(\theta_2) & 0 \\ 0 & 0 & \cos(\theta_3) \end{pmatrix}, \quad -M_2 = \begin{pmatrix} -\sin(\theta_1) & \cos(\theta_1) & 0 \\ -\sin(\theta_2) & -\cos(\theta_2) & 0 \\ 0 & 0 & -\sin(\theta_3) \end{pmatrix}$$

Let $\theta_k = \frac{2\pi x_k}{M}$. We define the 7-dimensional query vector \mathbf{q}_i and key vectors $\mathbf{k}_{j_1}, \mathbf{k}'_{j_2}$ via an input MLP ϕ and matrices Q, K, K' . Let c be a large scaling constant.

The 7-dimensional query vector $\mathbf{q}_i = Q\phi(x_i)$ is defined as:

$$\mathbf{q}_i = (c \cos(\theta_i), c \sin(\theta_i), 0, -c \sin(\theta_i), c \cos(\theta_i), 0, c)$$

The key vectors $\mathbf{k}_{j_1} = K\phi(x_{j_1})$ and $\mathbf{k}'_{j_2} = K'\phi(x_{j_2})$ for regular tokens are defined as:

$$\mathbf{k}_{j_1} = (\sin(\theta_{j_1}), \cos(\theta_{j_1}), 0, -\sin(\theta_{j_1}), -\cos(\theta_{j_1}), 0, 0)$$

$$\mathbf{k}'_{j_2} = (0, 0, \cos(\theta_{j_2}), 0, 0, -\sin(\theta_{j_2}), 0)$$

The attention score is computed via a hybrid mechanism:

1. **For regular pairs** (j_1, j_2) , the score is the sum of determinants of two 3D chunks formed from the first 6 dimensions of the vectors. The 7th dimension of the keys is 0, so it is ignored in this term.

$$\begin{aligned} A_{i,j_1,j_2} &= \det(\mathbf{q}_i[:3], \mathbf{k}_{j_1}[:3], \mathbf{k}'_{j_2}[:3]) + \det(\mathbf{q}_i[3:6], \mathbf{k}_{j_1}[3:6], \mathbf{k}'_{j_2}[3:6]) \\ &= c \cdot (\det(M_1) + \det(-M_2)) \quad (\text{from (21)}) \\ &= c \cdot \cos\left(\frac{2\pi(x_i + x_{j_1} + x_{j_2})}{M}\right) \quad (\text{since } \theta_i = 2\pi x_k/M), \end{aligned}$$

where $\mathbf{q}_i[l:l+m] = \{(\mathbf{q}_i)_l, \dots, (\mathbf{q}_i)_{l+m-1}\}$, denotes array slicing.

2. **For the blank pair**, the score is computed using the 7th dimension. It is the dot product of the query vector \mathbf{q}_i and a fixed key vector $\mathbf{k}_{\text{blank}} = (0, 0, 0, 0, 0, 0, 1)$:

$$A_{i,\text{blank}} = \mathbf{q}_i \cdot \mathbf{k}_{\text{blank}} = c$$

As a result, the attention score is maximized to a value of c if and only if $x_i + x_{j_1} + x_{j_2} = 0 \pmod{M}$. The blank pair also receives a score of c . For any non-matching triple, the score is strictly less than c .

The value vectors are defined by matrices V and V' .

- For any **regular token** x_j , we set its value embeddings to be $V\phi(x_j) = 1$ and $V'\phi(x_j) = 1$. The resulting value for the pair (j_1, j_2) in the final value matrix is their Kronecker product, which is 1.
- For the **blank pair**, the corresponding value is 0.

Let β_i be the number of pairs (j_1, j_2) that form a match with x_i . The softmax function distributes the attention weight almost exclusively among the entries with a score of c .

- If no match exists ($\beta_i = 0$), the blank pair receives all the attention, and the output is ≈ 0 since its value is 0.

- If at least one match exists ($\beta_i \geq 1$), the attention is distributed among the β_i matching pairs and the 1 blank pair. The output of the attention layer will be approximately $\frac{\beta_i \cdot (1) + 1 \cdot (0)}{\beta_i + 1} = \frac{\beta_i}{\beta_i + 1}$.

The final step is to design an output MLP ψ such that $\psi(z) = 1$ if $z \geq 1/2$ and $\psi(z) = 0$ otherwise, which is straightforward to implement.

B TRITON KERNEL: FORWARD PASS FOR 2-SIMPLICIAL ATTENTION

```

1 @triton.autotune(
2     configs=[
3         Config(
4             {
5                 "BLOCK_SIZE_Q": 64,
6                 "BLOCK_SIZE_KV": 32,
7                 "num_stages": 1,
8             },
9             num_warps=4,
10        )
11    ],
12    key=["HEAD_DIM"],
13 )
14 @triton.jit
15 def two_simplicial_attn_fwd_kernel(
16     Q_ptr, # [b, s, k, h]
17     K1_ptr, # [b, s, k, h]
18     K2_ptr, # [b, s, k, h]
19     V1_ptr, # [b, s, k, h]
20     V2_ptr, # [b, s, k, h]
21     O_ptr, # [b, s, k, h]
22     M_ptr, # [b, k, s]
23     bs,
24     seq_len,
25     num_heads,
26     head_dim,
27     w1: tl.constexpr,
28     w2: tl.constexpr,
29     q_stride_b,
30     q_stride_s,
31     q_stride_k,
32     q_stride_h,
33     k1_stride_b,
34     k1_stride_s,
35     k1_stride_k,
36     k1_stride_h,
37     k2_stride_b,
38     k2_stride_s,
39     k2_stride_k,
40     k2_stride_h,
41     v1_stride_b,
42     v1_stride_s,
43     v1_stride_k,
44     v1_stride_h,
45     v2_stride_b,
46     v2_stride_s,
47     v2_stride_k,
48     v2_stride_h,
49     out_stride_b,
50     out_stride_s,
51     out_stride_k,
52     out_stride_h,
53     m_stride_b,

```



```

54     m_stride_k,
55     m_stride_s,
56     BLOCK_SIZE_Q: tl.constexpr,
57     BLOCK_SIZE_KV: tl.constexpr,
58     HEAD_DIM: tl.constexpr,
59     INPUT_PRECISION: tl.constexpr,
60     SM_SCALE: tl.constexpr,
61     K2_BIAS: tl.constexpr,
62     V2_BIAS: tl.constexpr,
63     num_stages: tl.constexpr,
64 ):
65     data_dtype = tl.bfloat16
66     compute_dtype = tl.float32
67     gemm_dtype = tl.bfloat16
68
69     q_start = tl.program_id(0) * BLOCK_SIZE_Q
70     q_end = q_start + BLOCK_SIZE_Q
71     bk = tl.program_id(1)
72     offs_b = bk // num_heads
73     offs_k = bk % num_heads
74
75     qkv_offs_bk = offs_b * q_stride_b + offs_k * q_stride_k
76
77     Q_ptr += qkv_offs_bk
78     K1_ptr += qkv_offs_bk
79     K2_ptr += qkv_offs_bk
80     V1_ptr += qkv_offs_bk
81     V2_ptr += qkv_offs_bk
82     O_ptr += qkv_offs_bk
83     M_ptr += offs_b * m_stride_b + offs_k * m_stride_k
84
85     m_i = tl.zeros((BLOCK_SIZE_Q,), dtype=compute_dtype) - float("inf")
86     l_i = tl.zeros((BLOCK_SIZE_Q,), dtype=compute_dtype)
87     acc = tl.zeros((BLOCK_SIZE_Q, HEAD_DIM), dtype=compute_dtype)
88
89     q_offs_s = q_start + tl.arange(0, BLOCK_SIZE_Q)
90     qkv_offs_h = tl.arange(0, HEAD_DIM)
91     q_mask_s = q_offs_s < seq_len
92     qkv_mask_h = qkv_offs_h < head_dim
93     q_offs = q_offs_s[:, None] * q_stride_s + qkv_offs_h[None, :] *
94         q_stride_h
95     q_mask = q_mask_s[:, None] & (qkv_mask_h[None, :])
96
97     q_tile = tl.load(Q_ptr + q_offs, mask=q_mask).to(
98         compute_dtype
99     ) # [BLOCK_SIZE_Q, HEAD_DIM]
100     softmax_scale = tl.cast(SM_SCALE, gemm_dtype)
101
102     for kv1_idx in tl.range(tl.maximum(0, q_start - w1), tl.minimum(
103         seq_len, q_end)):
104         k1_offs = kv1_idx * k1_stride_s + qkv_offs_h * k1_stride_h
105         k1_tile = (tl.load(K1_ptr + k1_offs, mask=qkv_mask_h).to(
106             compute_dtype))[
107             None, :
108         ] # [1, HEAD_DIM]
109         qk1 = q_tile * k1_tile # [BLOCK_SIZE_Q, HEAD_DIM]
110         qk1 = qk1.to(gemm_dtype)
111
112         v1_offs = kv1_idx * v1_stride_s + qkv_offs_h * v1_stride_h
113         v1_tile = (tl.load(V1_ptr + v1_offs, mask=qkv_mask_h).to(
114             compute_dtype))[
115             None, :
116         ] # [1, HEAD_DIM]
117         for kv2_idx in tl.range(

```

```

115         tl.maximum(0, q_start - w2),
116         tl.minimum(seq_len, q_end),
117         BLOCK_SIZE_KV,
118         num_stages=num_stages,
119     ):
120         kv2_offs_s = kv2_idx + tl.arange(0, BLOCK_SIZE_KV)
121         kv2_mask_s = kv2_offs_s < seq_len
122         k2t_mask = kv2_mask_s[None, :] & qkv_mask_h[:, None]
123         v2_mask = kv2_mask_s[:, None] & qkv_mask_h[None, :]
124         k2_offs = (
125             kv2_offs_s[None, :] * k2_stride_s + qkv_offs_h[:, None] *
126             k2_stride_h
127         )
128         v2_offs = (
129             kv2_offs_s[:, None] * v2_stride_s + qkv_offs_h[None, :] *
130             v2_stride_h
131         )
132         k2t_tile = tl.load(K2_ptr + k2_offs, mask=k2t_mask).to(
133             compute_dtype
134         ) # [HEAD_DIM, BLOCK_SIZE_KV]
135         v2_tile = tl.load(V2_ptr + v2_offs, mask=v2_mask).to(
136             compute_dtype
137         ) # [BLOCK_SIZE_KV, HEAD_DIM]
138         k2t_tile += K2_BIAS
139         v2_tile += V2_BIAS
140         k2t_tile = k2t_tile.to(gemm_dtype)
141         v2_tile = v2_tile.to(compute_dtype)
142
143         qk = tl.dot(
144             qk1 * softmax_scale,
145             k2t_tile,
146             input_precision="tf32", # INPUT_PRECISION,
147             out_dtype=tl.float32,
148         ) # [BLOCK_SIZE_Q, BLOCK_SIZE_KV]
149
150         qk_mask = q_mask_s[:, None] & kv2_mask_s[None, :]
151         # Mask for q_idx - w1 < kv1_idx <= q_idx
152         # and q_idx - w2 < kv2_offs_s <= q_idx
153         kv1_local_mask = ((q_offs_s[:, None] - w1) < kv1_idx) & (
154             kv1_idx <= q_offs_s[:, None]
155         )
156         kv2_local_mask = ((q_offs_s[:, None] - w2) < kv2_offs_s[None,
157             :]) & (
158             kv2_offs_s[None, :] <= q_offs_s[:, None]
159         )
160         qk_mask &= kv1_local_mask & kv2_local_mask
161         qk += tl.where(qk_mask, 0, -1.0e38)
162
163         m_ij = tl.maximum(m_i, tl.max(qk, 1))
164         p = tl.math.exp(qk - m_ij[:, None])
165         l_ij = tl.sum(p, 1)
166         alpha = tl.math.exp(m_i - m_ij)
167         l_i = l_i * alpha + l_ij
168         acc = acc * alpha[:, None]
169
170         v12_tile = v1_tile * v2_tile # [BLOCK_SIZE_KV, HEAD_DIM]
171         acc += tl.dot(
172             p.to(gemm_dtype),
173             v12_tile.to(gemm_dtype),
174             input_precision="ieee", # INPUT_PRECISION,
175             out_dtype=tl.float32,
176         )
177
178         m_i = m_ij
179         acc = acc / l_i[:, None]

```

```

177     acc = tl.where(q_mask, acc, 0.0)
178     acc = acc.to(data_dtype)
179     out_offs = q_offs_s[:, None] * out_stride_s + qkv_offs_h[None, :] *
180         out_stride_h
181     tl.store(O_ptr + out_offs, acc, mask=q_mask)
182
183     m = m_i + tl.log(l_i)
184
185     m_offs = q_offs_s * m_stride_s
186     m_mask = q_offs_s < seq_len
187     tl.store(M_ptr + m_offs, m, mask=m_mask)

```

Listing 1: Forward pass for 2-simplicial attention.

C TRITON KERNEL: BACKWARD PASS FOR 2-SIMPLICIAL ATTENTION

```

1 @triton.jit
2 def two_simplicial_attn_bwd_kv1_kernel(
3     Q_ptr, # [b, s, k, h]
4     K1_ptr, # [b, s, k, h]
5     K2_ptr, # [b, s, k, h]
6     V1_ptr, # [b, s, k, h]
7     V2_ptr, # [b, s, k, h]
8     dO_ptr, # [b, s, k, h]
9     M_ptr, # [b, k, s]
10    D_ptr, # [b, k, s]
11    dQ_ptr, # [b, s, k, h]
12    dK1_ptr, # [b, s, k, h]
13    dV1_ptr, # [b, s, k, h]
14    # Skip writing dk2, dv2 for now.
15    bs,
16    seq_len,
17    num_heads,
18    head_dim,
19    w1, # Q[i]: KV1(i-w1,i]
20    w2, # Q[i]: KV2(i-w2,i]
21    q_stride_b,
22    q_stride_s,
23    q_stride_k,
24    q_stride_h,
25    k1_stride_b,
26    k1_stride_s,
27    k1_stride_k,
28    k1_stride_h,
29    k2_stride_b,
30    k2_stride_s,
31    k2_stride_k,
32    k2_stride_h,
33    v1_stride_b,
34    v1_stride_s,
35    v1_stride_k,
36    v1_stride_h,
37    v2_stride_b,
38    v2_stride_s,
39    v2_stride_k,
40    v2_stride_h,
41    dO_stride_b,
42    dO_stride_s,
43    dO_stride_k,
44    dO_stride_h,
45    m_stride_b,
46    m_stride_k,

```

```

47     m_stride_s,
48     d_stride_b,
49     d_stride_k,
50     d_stride_s,
51     dq_stride_b,
52     dq_stride_s,
53     dq_stride_k,
54     dq_stride_h,
55     dkl_stride_b,
56     dkl_stride_s,
57     dkl_stride_k,
58     dkl_stride_h,
59     dvl_stride_b,
60     dvl_stride_s,
61     dvl_stride_k,
62     dvl_stride_h,
63     BLOCK_SIZE_Q: tl.constexpr,
64     BLOCK_SIZE_KV: tl.constexpr,
65     HEAD_DIM: tl.constexpr,
66     SM_SCALE: tl.constexpr,
67     K2_BIAS: tl.constexpr,
68     V2_BIAS: tl.constexpr,
69     COMPUTE_DQ: tl.constexpr,
70     num_stages: tl.constexpr,
71     is_flipped: tl.constexpr,
72 ):
73     data_dtype = tl.bfloat16
74     compute_dtype = tl.float32
75     gemm_dtype = tl.bfloat16
76
77     kv1_start = tl.program_id(0) * BLOCK_SIZE_KV
78     kv1_end = kv1_start + BLOCK_SIZE_KV
79     bk = tl.program_id(1)
80     offs_b = bk // num_heads
81     offs_k = bk % num_heads
82
83     qkv_offs_bk = offs_b * q_stride_b + offs_k * q_stride_k
84     Q_ptr += qkv_offs_bk
85     K1_ptr += qkv_offs_bk
86     K2_ptr += qkv_offs_bk
87     V1_ptr += qkv_offs_bk
88     V2_ptr += qkv_offs_bk
89
90     dO_ptr += offs_b * dO_stride_b + offs_k * dO_stride_k
91     M_ptr += offs_b * m_stride_b + offs_k * m_stride_k
92     D_ptr += offs_b * d_stride_b + offs_k * d_stride_k
93     dK1_ptr += offs_b * dkl_stride_b + offs_k * dkl_stride_k
94     dV1_ptr += offs_b * dvl_stride_b + offs_k * dvl_stride_k
95     if COMPUTE_DQ:
96         dQ_ptr += offs_b * dq_stride_b + offs_k * dq_stride_k
97
98     softmax_scale = tl.cast(SM_SCALE, gemm_dtype)
99     qkv_offs_h = tl.arange(0, HEAD_DIM)
100     qkv_mask_h = qkv_offs_h < head_dim
101
102     kv1_offs_s = kv1_start + tl.arange(0, BLOCK_SIZE_KV)
103
104     k1_offs = kv1_offs_s[:, None] * k1_stride_s + qkv_offs_h[None, :] *
        k1_stride_h
105     kv1_mask_s = kv1_offs_s < seq_len
106     kv1_mask = kv1_mask_s[:, None] & qkv_mask_h[None, :]
107     k1_tile = tl.load(K1_ptr + k1_offs, mask=kv1_mask).to(
        compute_dtype
108 ) # [BLOCK_SIZE_KV, HEAD_DIM]

```

```

110     vl_offs = kv1_offs_s[:, None] * vl_stride_s + qkv_offs_h[None, :] *
        vl_stride_h
111     vl_tile = tl.load(Vl_ptr + vl_offs, mask=kv1_mask).to(
112         compute_dtype
113     ) # [BLOCK_SIZE_KV, HEAD_DIM]
114     if is_flipped:
115         k1_tile += K2_BIAS
116         v1_tile += V2_BIAS
117     dv1 = tl.zeros((BLOCK_SIZE_KV, HEAD_DIM), compute_dtype)
118     dk1 = tl.zeros((BLOCK_SIZE_KV, HEAD_DIM), compute_dtype)
119     # for kv2_idx in tl.range(0, seq_len):
120     # kv1 - w2 < kv2 <= kv1 + w1
121     for kv2_idx in tl.range(
122         tl.maximum(0, kv1_start - w2), tl.minimum(seq_len, kv1_end + w1)
123     ):
124         k2_offs = kv2_idx * k2_stride_s + qkv_offs_h * k2_stride_h
125         k2_tile = (tl.load(K2_ptr + k2_offs, mask=qkv_mask_h).to(
126             compute_dtype))[
127             None, :
128         ] # [1, HEAD_DIM]
129         v2_offs = kv2_idx * v2_stride_s + qkv_offs_h * v2_stride_h
130         v2_tile = (tl.load(V2_ptr + v2_offs, mask=qkv_mask_h).to(
131             compute_dtype))[
132             None, :
133         ] # [1, HEAD_DIM]
134         if not is_flipped:
135             k2_tile += K2_BIAS
136             v2_tile += V2_BIAS
137         k1k2 = k1_tile * k2_tile # [BLOCK_SIZE_KV, HEAD_DIM]
138         v1v2 = v1_tile * v2_tile # [BLOCK_SIZE_KV, HEAD_DIM]
139         k1k2 = k1k2.to(gemm_dtype)
140         v1v2 = v1v2.to(gemm_dtype)
141         # kv1 <= q < kv1 + w1
142         # kv2 <= q < kv2 + w2
143         q_start = tl.maximum(kv1_start, kv2_idx)
144         q_end = tl.minimum(seq_len, tl.minimum(kv1_end + w1, kv2_idx + w2))
145         for q_idx in tl.range(q_start, q_end, BLOCK_SIZE_Q):
146             # Load qt, m, d, dO
147             q_offs_s = q_idx + tl.arange(0, BLOCK_SIZE_Q)
148             q_offs = q_offs_s[None, :] * q_stride_s + qkv_offs_h[:, None]
149             * q_stride_h
150             q_mask_s = q_offs_s < seq_len
151             qt_mask = q_mask_s[None, :] & qkv_mask_h[:, None]
152             qt_tile = tl.load(Q_ptr + q_offs, mask=qt_mask).to(
153                 gemm_dtype
154             ) # [HEAD_DIM, BLOCK_SIZE_Q]
155             m_offs = q_offs_s * m_stride_s
156             m_tile = tl.load(M_ptr + m_offs, mask=q_mask_s).to(
157                 compute_dtype)[
158                 None, :
159             ] # [1, BLOCK_SIZE_Q]
160             d_offs = q_offs_s * d_stride_s
161             d_tile = tl.load(D_ptr + d_offs, mask=q_mask_s).to(
162                 compute_dtype)[
163                 None, :
164             ] # [1, BLOCK_SIZE_Q]
165             dO_offs = (
166                 q_offs_s[:, None] * dO_stride_s + qkv_offs_h[None, :] *
167                 dO_stride_h
168             )
169             dO_tile = tl.load(
170                 dO_ptr + dO_offs, mask=q_mask_s[:, None] & qkv_mask_h[
171                     None, :]
172             ).to(compute_dtype) # [BLOCK_SIZE_Q, HEAD_DIM]

```

```

166         if COMPUTE_DQ:
167             dq = tl.zeros((BLOCK_SIZE_Q, HEAD_DIM), tl.float32)
168             # Compute dvl.
169             # [KV, D] @ [D, Q] => [KV, Q]
170             qkkT = tl.dot(
171                 k1k2, qt_tile * softmax_scale, out_dtype=tl.float32
172             ) # [BLOCK_SIZE_KV, BLOCK_SIZE_Q]
173
174             # Mask qkkT to -inf.
175             kv1_local_mask = ((q_offs_s[None, :] - w1) < kv1_offs_s[:,
176                 None]) & (
177                 kv1_offs_s[:, None] <= q_offs_s[None, :])
178             kv2_local_mask = ((q_offs_s - w2) < kv2_idx) & (kv2_idx <=
179                 q_offs_s)
180             local_mask = (
181                 kv1_local_mask & kv2_local_mask[None, :])
182             qkkT = tl.where(local_mask, qkkT, -1.0e38)
183
184             pT = tl.exp(qkkT - m_tile) # [BLOCK_SIZE_KV, BLOCK_SIZE_Q]
185             pT = tl.where(local_mask, pT, 0.0)
186             dOv2 = dO_tile * v2_tile # [BLOCK_SIZE_Q, HEAD_DIM]
187             dvl += tl.dot(
188                 pT.to(gemm_dtype), dOv2.to(gemm_dtype), out_dtype=tl.
189                 float32
190             ) # [BLOCK_SIZE_KV, HEAD_DIM]
191
192             dpT = tl.dot(
193                 v1v2, tl.trans(dO_tile.to(gemm_dtype)), out_dtype=tl.
194                 float32
195             ) # [BLOCK_SIZE_KV, BLOCK_SIZE_Q]
196             dsT = pT * (dpT - d_tile) # [BLOCK_SIZE_KV, BLOCK_SIZE_Q]
197             dsT = tl.where(local_mask, dsT, 0.0)
198             dsT = dsT.to(gemm_dtype)
199
200             dk1 += (
201                 tl.dot(dsT, tl.trans(qt_tile), out_dtype=tl.float32)
202                 * k2_tile.to(tl.float32)
203                 * softmax_scale
204             )
205             if COMPUTE_DQ:
206                 # dq[q, d] = dsT.T[q, kv1] @ k1k2[kv1, d]
207                 dq += (
208                     tl.dot(tl.trans(dsT), k1k2, out_dtype=tl.float32) *
209                     softmax_scale
210                 ) # [BLOCK_SIZE_Q, HEAD_DIM]
211                 dq_offs = (
212                     q_offs_s[:, None] * dq_stride_s + qkv_offs_h[None, :]
213                     * dq_stride_h
214                 )
215                 tl.atomic_add(
216                     dQ_ptr + dq_offs, dq, mask=q_mask_s[:, None] &
217                     qkv_mask_h[None, :])
218
219             dvl_offs = kv1_offs_s[:, None] * dvl_stride_s + qkv_offs_h[None, :] *
220                 dvl_stride_h
221             dk1_offs = kv1_offs_s[:, None] * dk1_stride_s + qkv_offs_h[None, :] *
222                 dk1_stride_h
223             tl.store(dvl_ptr + dvl_offs, dvl.to(data_dtype), mask=kv1_mask)
224             tl.store(dk1_ptr + dk1_offs, dk1.to(data_dtype), mask=kv1_mask)

```

Listing 2: Backward pass for 2-simplicial attention.

```

1 @triton.autotune(
2     configs=[
3         Config(
4             {
5                 "BLOCK_SIZE_Q": 32,
6                 "BLOCK_SIZE_KV2": 64,
7                 "num_stages": 1,
8             },
9             num_warps=4,
10        )
11    ],
12    key=["HEAD_DIM"],
13 )
14 @triton.jit
15 def two_simplicial_attn_bwd_kv2q_kernel(
16     Q_ptr, # [b, s, k, h]
17     K1_ptr, # [b, s, k, h]
18     K2_ptr, # [b, s, k, h]
19     V1_ptr, # [b, s, k, h]
20     V2_ptr, # [b, s, k, h]
21     dO_ptr, # [b, s, k, h]
22     M_ptr, # [b, k, s]
23     D_ptr, # [b, k, s]
24     dQ_ptr, # [b, s, k, h]
25     dK2_ptr, # [b, s, k, h]
26     dV2_ptr, # [b, s, k, h]
27     bs,
28     seq_len,
29     num_heads,
30     head_dim,
31     w1, # Q[i]: KV1(i-w1,i]
32     w2, # Q[i]: KV2(i-w2,i]
33     q_stride_b,
34     q_stride_s,
35     q_stride_k,
36     q_stride_h,
37     k1_stride_b,
38     k1_stride_s,
39     k1_stride_k,
40     k1_stride_h,
41     k2_stride_b,
42     k2_stride_s,
43     k2_stride_k,
44     k2_stride_h,
45     v1_stride_b,
46     v1_stride_s,
47     v1_stride_k,
48     v1_stride_h,
49     v2_stride_b,
50     v2_stride_s,
51     v2_stride_k,
52     v2_stride_h,
53     dO_stride_b,
54     dO_stride_s,
55     dO_stride_k,
56     dO_stride_h,
57     m_stride_b,
58     m_stride_k,
59     m_stride_s,
60     d_stride_b,
61     d_stride_k,
62     d_stride_s,
63     dq_stride_b,
64     dq_stride_s,
65     dq_stride_k,

```



```

66     dq_stride_h,
67     dk2_stride_b,
68     dk2_stride_s,
69     dk2_stride_k,
70     dk2_stride_h,
71     dv2_stride_b,
72     dv2_stride_s,
73     dv2_stride_k,
74     dv2_stride_h,
75     BLOCK_SIZE_Q: tl.constexpr,
76     BLOCK_SIZE_KV2: tl.constexpr,
77     HEAD_DIM: tl.constexpr,
78     SM_SCALE: tl.constexpr,
79     K2_BIAS: tl.constexpr,
80     V2_BIAS: tl.constexpr,
81     num_stages: tl.constexpr,
82     IS_SECOND_PASS: tl.constexpr,
83 ):
84     assert BLOCK_SIZE_KV2 == BLOCK_SIZE_Q + w2
85     data_dtype = tl.bfloat16
86     compute_dtype = tl.float32
87     gemm_dtype = tl.bfloat16
88
89     # First pass does even tiles, second pass does odd tiles.
90     q_start = tl.program_id(0) * BLOCK_SIZE_KV2
91     if IS_SECOND_PASS:
92         q_start += BLOCK_SIZE_Q
93     q_end = q_start + BLOCK_SIZE_Q
94     kv2_start = q_start - w2
95
96     bk = tl.program_id(1)
97     offs_b = bk // num_heads
98     offs_k = bk % num_heads
99
100     qkv_offs_bk = offs_b * q_stride_b + offs_k * q_stride_k
101     Q_ptr += qkv_offs_bk
102     K1_ptr += qkv_offs_bk
103     K2_ptr += qkv_offs_bk
104     V1_ptr += qkv_offs_bk
105     V2_ptr += qkv_offs_bk
106
107     dO_ptr += offs_b * dO_stride_b + offs_k * dO_stride_k
108     M_ptr += offs_b * m_stride_b + offs_k * m_stride_k
109     D_ptr += offs_b * d_stride_b + offs_k * d_stride_k
110     dQ_ptr += offs_b * dq_stride_b + offs_k * dq_stride_k
111     dk2_ptr += offs_b * dk2_stride_b + offs_k * dk2_stride_k
112     dv2_ptr += offs_b * dv2_stride_b + offs_k * dv2_stride_k
113
114     softmax_scale = tl.cast(SM_SCALE, gemm_dtype)
115     qkv_offs_h = tl.arange(0, HEAD_DIM)
116     qkv_mask_h = qkv_offs_h < head_dim
117
118     q_offs_s = q_start + tl.arange(0, BLOCK_SIZE_Q)
119     kv2_offs_s = kv2_start + tl.arange(0, BLOCK_SIZE_KV2)
120     q_offs = q_offs_s[:, None] * q_stride_s + qkv_offs_h[None, :] *
        q_stride_h
121     kv2_offs = kv2_offs_s[:, None] * k2_stride_s + qkv_offs_h[None, :] *
        k2_stride_h
122     m_offs = q_offs_s * m_stride_s
123     d_offs = q_offs_s * d_stride_s
124     dO_offs = q_offs_s[:, None] * dO_stride_s + qkv_offs_h[None, :] *
        dO_stride_h
125     q_mask_s = q_offs_s < seq_len
126     q_mask = q_mask_s[:, None] & qkv_mask_h[None, :]
127     kv2_mask_s = 0 <= kv2_offs_s and kv2_offs_s < seq_len

```

```

128 kv2_mask = kv2_mask_s[:, None] & qkv_mask_h[None, :]
129
130
131 q_tile = tl.load(Q_ptr + q_offs, mask=q_mask).to(
132     compute_dtype
133 ) # [BLOCK_SIZE_Q, HEAD_DIM]
134 k2_tile = tl.load(K2_ptr + kv2_offs, mask=kv2_mask).to(gemm_dtype) #
135     [KV2, HEAD_DIM]
136 v2_tile = tl.load(V2_ptr + kv2_offs, mask=kv2_mask).to(gemm_dtype) #
137     [KV2, HEAD_DIM]
138 m_tile = tl.load(M_ptr + m_offs, mask=q_mask_s).to(compute_dtype) # [
139     BLOCK_SIZE_Q]
140 d_tile = tl.load(D_ptr + d_offs, mask=q_mask_s).to(compute_dtype) # [
141     BLOCK_SIZE_Q]
142 dO_tile = tl.load(dO_ptr + dO_offs, mask=q_mask).to(
143     gemm_dtype
144 ) # [BLOCK_SIZE_Q, HEAD_DIM]
145
146 # Apply KV2 norm.
147 k2_tile += K2_BIAS
148 v2_tile += V2_BIAS
149 k2_tile = k2_tile.to(gemm_dtype)
150 v2_tile = v2_tile.to(gemm_dtype)
151
152 dq = tl.zeros((BLOCK_SIZE_Q, HEAD_DIM), tl.float32)
153 dk2 = tl.zeros((BLOCK_SIZE_KV2, HEAD_DIM), tl.float32)
154 dv2 = tl.zeros((BLOCK_SIZE_KV2, HEAD_DIM), tl.float32)
155
156 kv1_start = tl.maximum(0, q_start - w1)
157 kv1_end = tl.minimum(seq_len, q_end)
158 for kv1_idx in tl.range(kv1_start, kv1_end, num_stages=num_stages):
159     k1_offs = kv1_idx * k1_stride_s + qkv_offs_h * k1_stride_h
160     v1_offs = kv1_idx * v1_stride_s + qkv_offs_h * v1_stride_h
161     k1_tile = tl.load(K1_ptr + k1_offs, mask=qkv_mask_h).to(
162         compute_dtype
163     ) # [HEAD_DIM]
164
165     v1_tile = tl.load(V1_ptr + v1_offs, mask=qkv_mask_h).to(
166         compute_dtype
167     ) # [HEAD_DIM]
168
169     qk1_s = q_tile * (k1_tile[None, :] * softmax_scale) # [Q, D]
170     qk1_s = qk1_s.to(gemm_dtype)
171     # k2[KV, Q] @ qk1_s.T[Q, D] => [KV2, Q]
172     qkkT = tl.dot(k2_tile, qk1_s.T, out_dtype=tl.float32) # [KV2, Q]
173
174     qkT_mask = kv2_mask_s[:, None] & q_mask_s[None, :]
175     kv1_local_mask = ((q_offs_s[None, :] - w1) < kv1_idx) & (
176         kv1_idx <= q_offs_s[None, :])
177     ) # [KV2, Q]
178     kv2_local_mask = ((q_offs_s[None, :] - w2) < kv2_offs_s[:, None])
179     & (
180         kv2_offs_s[:, None] <= q_offs_s[None, :])
181     ) # [KV2, Q]
182     local_mask = (
183         kv1_local_mask & kv2_local_mask
184     ) # [BLOCK_SIZE_KV, BLOCK_SIZE_Q]
185     qkT_mask &= kv1_local_mask & kv2_local_mask
186
187     pT = tl.exp(qkkT - m_tile[None, :]) # [KV2, Q]
188     pT = tl.where(qkT_mask, pT, 0.0)
189
190     qkkT = tl.where(local_mask, qkkT, -1.0e38)
191
192     dOv1 = dO_tile * v1_tile[None, :] # [Q, D]

```

```

188     dOv1 = dOv1.to(gemm_dtype)
189     # pT[KV2, Q] @ dOv1[Q, D] => [KV2, D]
190     dv2 += tl.dot(pT.to(gemm_dtype), dOv1, out_dtype=tl.float32)
191
192     # v2[KV2, D] @ dOv1.T[D, Q] => dpT[KV2, Q]
193     dpT = tl.dot(v2_tile, dOv1.T, out_dtype=tl.float32)
194     dsT = pT * (dpT - d_tile[None, :]) # [KV2, Q]
195     dsT = tl.where(qkT_mask, dsT, 0.0)
196     dsT = dsT.to(gemm_dtype) # [KV2, Q]
197
198     # dsT[KV2, Q] @ qk1[Q, D] => dk2[KV2, D]
199     dk2 += tl.dot(dsT, qk1_s, out_dtype=tl.float32)
200
201     k1k2 = k1_tile[None, :] * k2_tile # [KV2, D]
202     k1k2 = k1k2.to(gemm_dtype)
203
204     dq += tl.dot(dsT.T, k1k2) # * softmax scale at the end.
205
206     # End. update derivatives.
207     if IS_SECOND_PASS:
208         #load, add.
209         prev_dk2 = tl.load(dK2_ptr + kv2_offs, kv2_mask)
210         prev_dv2 = tl.load(dV2_ptr + kv2_offs, kv2_mask)
211         dk2 += prev_dk2
212         dv2 += prev_dv2
213
214     dq *= softmax_scale
215     tl.store(dK2_ptr + kv2_offs, dk2, kv2_mask)
216     tl.store(dV2_ptr + kv2_offs, dv2, kv2_mask)
217     tl.store(dQ_ptr + q_offs, dq, q_mask)

```

Listing 3: Backward pass for 2-simplicial attention optimized for small w_2 avoiding atomic adds.